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by

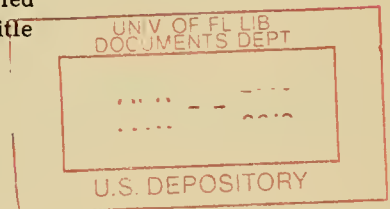
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CALCULATION OF NEUTRON DISTRIBUTIONS IN HETEROGENEOUS PILES

By A. M. Weinberg

The calculation of the slow neutron density in a pile which consists of lumps of uranium disposed in a lattice is a problem of fundamental importance in elementary pile theory. The method used for such a calculation is rather similar to the method used for calculating the distribution around control rods; it is therefore doubly worthwhile to examine the calculation in detail.

In a thermal neutron heterogeneous pile, fast neutrons produced as the result of fission in the uranium lumps are moderated by, for example, the graphite matrix in which the rods are embedded until they become slow. The neutrons then diffuse in accordance with laws of diffusion theory until they are finally captured in the moderator, or in the uranium, or until they escape from the boundaries of the pile.

We consider an infinite prototype of an actual pile. Our problem is to calculate the fraction of the thermal neutrons absorbed inside this infinite pile which are absorbed in the uranium. We call the ratio:

$$\frac{\text{neutrons absorbed in uranium}}{\text{neutrons absorbed in uranium and moderator}}$$

the thermal utilization; in accordance with usual practice we denote this quantity of f_{∞} or simply f . The ratio of slow neutrons absorbed in uranium to neutrons produced in a finite pile, called the effective thermal utilization, and denoted by f_{eff} , is evidently less than the ratio of slow neutrons absorbed in uranium to slow neutrons produced as a result of slowing down—the reason being that not all slow neutrons produced are absorbed inside the pile. However, in pile theory, it is customary to first examine the infinite prototype of a pile, then to deal with the corrections introduced by the finiteness of the pile, i.e., it is customary to separate microscopic pile theory from macroscopic pile theory. It will be our purpose here to consider only the calculation of the thermal utilization in an infinite lattice. The thermal utilization in the finite lattice depends on the fraction of neutrons which escape from the pile, and therefore upon the size of the pile in which the lattice is placed. Its calculation is very much more difficult than the calculation of f .

The calculation of f according to elementary diffusion theory is very straightforward. The method and the assumptions are quite analogous to those used for the calculation of wave functions in crystal lattices. We list the assumptions as follows:

- 1) Elementary diffusion theory is applicable.
- 2) The production of thermal neutrons is uniform throughout the moderator, and is zero in the uranium.
- 3) The units cell of a lattice can be replaced by a sphere in case the lattice is a point lattice, e.g., simple cubic, or a cylinder in case the lattice is a rod lattice.

We now discuss the validity of these assumptions:

1) The assumption of elementary diffusion theory as is well known, is accurate first, if the dimensions of the system are large compared to a mean free path; second, if the system does not absorb neutrons very heavily and third, if the system contains no sources. None of these assumptions are strictly correct in a uranium lattice. The errors which are involved because elementary diffusion theory is used, can be estimated. It turns out that they are sizeable in lattices of interest but the labor involved in extending calculations to include the more accurate theory is prohibitive if a large number of calculations, such as are needed in calculating optimum lattice dimensions, are to be performed.

2) The assumption that thermal neutrons are produced uniformly throughout a cell is accurate if the cell size, i.e., the separation between lumps, is not large compared to a slowing down distance. It is easy to compute the slowing down density in an infinite lattice at each of whose points neutrons, which slow down according to a Gaussian picture, are produced. It is rather remarkable how uniform the slow neutron production rate is in such a lattice.

3) This procedure of replacing e.g., a cubic cell by a spherical one is called sphericizing of the unit cell; it is entirely analogous to the Wigner-Seitz method for calculating the first approximation to the wave functions in a crystal lattice. The sphericizing assumption is made essential in order to simplify the calculational procedure. Thus if the lattice is a simple cubic lattice the unit cell is a cube and the neutron distribution involves all spherical harmonics of order $4n$. The sphericizing approximation implies that only the spherical harmonic of zero order is considered. Evidently the nearer the actual cell is to the "sphericized" cell, the closer is the approximate neutron density to the actual one. In case the uranium is disposed in parallel plates, the "sphericized" cell and the actual cell are identical, both being defined by the planes of symmetry between the uranium plates.

The details of the calculation are now easy to write down. We must solve a simple diffusion equation for the thermal neutron density in the moderator and a similar diffusion equation in the uranium and must apply the appropriate boundary conditions at the boundary of the sphericized unit cell and at the interface between the uranium and the metal. Thus in the moderator we have the equation

$$\frac{N_1 \sigma_{a1}}{\kappa_1^2} \Delta \phi_1 - N_1 \sigma_{a1} \phi_1 + q = 0 \quad (1)$$

where ϕ_1 is the sum of the speeds of all the thermal neutrons in a cubic centimeter, $N_1 \sigma_{a1}$ is the macroscopic absorption cross section of the moderator, κ_1 is the reciprocal of the diffusion length in the moderator, and q is the number of thermal neutrons produced per cubic centimeter per second.

The quantity $\frac{N_1 \sigma_{a1}}{\kappa_1^2}$ is recognized as the diffusion coefficient according to the elementary diffusion theory. In the uranium a similar equation is written down, but since practically no neutrons are produced there, the uranium atomic weight being so large, it is appropriate to set $q = 0$. Thus in the uranium we have

$$\frac{N_0 \sigma_{a0}}{\kappa_0^2} \Delta \phi_0 - N_0 \sigma_{a0} \phi_0 = 0 \quad (2)$$

where the subscript zero refers to the uranium region. The cell we take to be either a composite sphere, a composite cylinder, or a composite slab (see Figure 1); in all cases we denote the one-half diameter of the uranium by r_0 , the one-half thickness of the cell by r_1 .

The boundary conditions at the interface between the uranium and the moderator, i.e., at $r = r_0$, must be continuity of flux and continuity of net current. (This corresponds to ensuring continuity of the first two harmonics in a spherical harmonic expansion of the slow neutron angular distribution.) The boundary conditions can therefore be written:

$$\frac{N_1 \sigma_{a1}}{\kappa_1^2} \frac{\partial \phi_1}{\partial \nu} = \frac{N_0 \sigma_{a0}}{\kappa_0^2} \frac{\partial \phi_0}{\partial \nu} \quad \text{at } r = r_0 \quad (3)$$

$$\phi_1 = \phi_0 \quad \text{at } r = r_0 \quad (4)$$

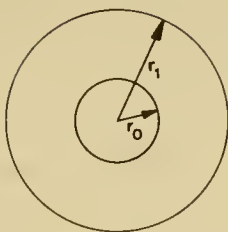


Figure 1.

where ν represents the outward normal. Finally, at the outer boundary of the cell there can be no net flow of neutrons, i.e.,

$$\frac{\partial \phi_1}{\partial \nu} = 0 \quad \text{at } r = r_1. \quad (5)$$

To solve these equations is straightforward. We set

$$\phi_0 = A Z_{01}(\kappa_0 r) \quad (6)$$

and

$$\phi_1 = \frac{q}{N_1 \sigma a_1} - B \left[Z'_{11}(\kappa_1 r_1) Z_{12}(\kappa_1 r) - Z_{11}(\kappa_1 r) Z'_{12}(\kappa_1 r_1) \right] \quad (7)$$

where A and B are arbitrary constants, $Z_{ij}(\kappa_1 r)$ is a function which solves the equation

$$\Delta Z_{ij} - \kappa_i^2 Z_{ij} = 0 \quad (8)$$

in the appropriate geometry and ' denotes derivative.

Since (8) is a second order differential equation it has two solutions which we distinguish by the subscript $j = 1$ or 2 . One of these solutions will be singular at the origin (in cylindrical or spherical geometry), or will be nonsymmetric about the origin (plane geometry). This function we denote by $j = 2$. The other function will be symmetric and nonsingular at the origin; this we denote by $j = 1$.

We tabulate the functions Z_{ij} and their derivatives for the three geometries in the following table:

The Functions Z_{ij}

Geometry	$Z_{11}(\kappa_i r)$	$Z'_{11}(\kappa_i r)$	$Z_{12}(\kappa_i r)$	$Z'_{12}(\kappa_i r)$
Plane	$\cosh \kappa_i r$	$\sinh \kappa_i r$	$\sinh \kappa_i r$	$\cosh \kappa_i r$
Cylinder	$I_0(\kappa_i r)$	$I_1(\kappa_i r)$	$K_0(\kappa_i r)$	$-K_1(\kappa_i r)$
Sphere	$\frac{\sinh \kappa_i r}{\kappa_i r}$	$\frac{\kappa_i r \cosh \kappa_i r - \sinh \kappa_i r}{(\kappa_i r)^2}$	$\frac{\cosh \kappa_i r}{\kappa_i r}$	$\frac{\kappa_i r \cosh \kappa_i r - \cosh \kappa_i r}{(\kappa_i r)^2}$

The linear combination of Z_{11} and Z_{12} chosen in (7) automatically satisfies boundary condition (5) i.e., no net current at the edge of the unit cell. There are still the two boundary conditions (3) and (4)

to be satisfied, and these two conditions are just enough to determine the arbitrary constants A and B. Substituting (6) and (7) into (3) and (4) we get the following pair of equations for A and B:

$$\begin{aligned} -B \frac{N_1 \sigma_{a1}}{\kappa_1} [Z'_{11}(\kappa_1 r_1) Z'_{12}(\kappa_1 r_0) + Z'_{11}(\kappa_1 r_0) Z'_{12}(\kappa_1 r_1)] \\ + A \frac{N_0 \sigma_{a0}}{\kappa_0} Z'_{01}(\kappa_0 r_0) = 0 \end{aligned} \quad (8)$$

$$\begin{aligned} B [Z'_{11}(\kappa_1 r_1) Z'_{12}(\kappa_1 r_0) - Z'_{11}(\kappa_1 r_0) Z'_{12}(\kappa_1 r_1)] \\ + A Z'_{01}(\kappa_0 r_0) = \frac{q \kappa_1^2}{N_1 a_1} \end{aligned} \quad (9)$$

from which we obtain $1/A$:

$$\frac{1}{A} = \frac{\frac{N_0 \sigma_{a0}}{\kappa_0} Z'_{01}(\kappa_0 r_0) C(\kappa_1 r_1, \kappa_1 r_0) + \frac{N_1 \sigma_{a1}}{\kappa_1} Z'_{01}(\kappa_0 r_0) C'(\kappa_1 r_1, \kappa_1 r_0)}{C'(\kappa_1 r_1, \kappa_1 r_0) q / \kappa_1} \quad (10)$$

where

$$C(x, y) = Z'_{11}(x) Z'_{12}(y) - Z'_{11}(y) Z'_{12}(x) \quad (11)$$

$$C'(x, y) = Z'_{11}(x) Z'_{12}(y) - Z'_{11}(y) Z'_{12}(x) \quad (12)$$

From the expression for A and the corresponding expression for B, the neutron fluxes (6) and (7) can be calculated. The general shape of the flux distributions are given in Figure 2. It is seen there that the density is highest in the moderator where the slow neutrons are produced, and dips in the uranium where the neutrons are absorbed but are not produced.

The thermal utilization is defined as the ratio of slow neutrons absorbed in the uranium to slow neutrons produced (by moderation) in the moderator. Since the number of neutrons absorbed in the uranium must equal the number which flow into the uranium

$$\frac{1}{f} = \frac{q_1 V_1}{\frac{N_0 \sigma_{a0}}{\kappa_0^2} S_0 \left. \frac{\partial \Phi_1}{\partial r} \right|_{r_0}} = \frac{q_1 V_1}{\frac{N_0 \sigma_{a0}}{\kappa_0^2} S_0 Z'_{01}(\kappa_0 r_0)} \frac{1}{A} \quad (13)$$

where S_0 is the surface of the uranium lump and V_1 is the volume of the moderator. We substitute (10) into (13), and use Gauss's theorem:

$$\begin{aligned} \bar{Z}_0 V_0 &= \int_{V_0} Z_{01}(\kappa_0 r) dV_0 = \frac{1}{\kappa_0^2} \int_{V_0} \Delta Z_{01}(\kappa_0 r) dV_0 = \frac{S_0 Z'_{01}(\kappa_0 r_0)}{\kappa_0} \\ \bar{C}_1 V_1 &= \int_{V_1} C_1(\kappa_1 r) dV_1 = \frac{1}{\kappa_1^2} \int_{V_1} \Delta C_1(\kappa_1 r) dV_1 = \frac{S_0 C'_1(\kappa_1 r_0)}{\kappa_1} \end{aligned}$$

where bar denotes average. Thus

$$\frac{1}{f} = \frac{N_1 \sigma_{a1} V_1}{N_0 \sigma_{a0} V_0} F + E = 1 + \frac{N_1 \sigma_{a1} V_1}{N_0 \sigma_{a0} V_0} F + E - 1 \quad (15)$$

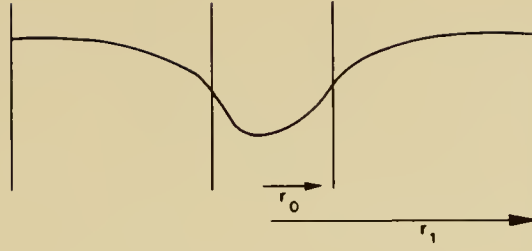


Figure 2.

where

$$F = \frac{\kappa_0 V_0}{S_0} \frac{Z_{01}(\kappa_0 r_0)}{Z_{01}'(\kappa_0 r_0)} = \frac{Z_{01}(\kappa_0 r_0)}{\bar{Z}_{01}'(\kappa_0 r_0)} \quad (16)$$

and

$$E = - \frac{\kappa_1 V_1}{S_0} \frac{C_1(\kappa_1 r_0, \kappa_1 r_1)}{C_1'(\kappa_1 r_0, \kappa_1 r_1)} = \frac{C_1(\kappa_1 r_0, \kappa_1 r_1)}{\bar{C}_1'(\kappa_1 r_0, \kappa_1 r_1)} \quad (17)$$

The actual formulas for F and C depend upon the geometry of the cell. We list these formulas in the following table:

Table of F and E

Plane	$\kappa_0 r_0 \coth \kappa_0 r_0$	$\kappa_1 (r_1 - r_0) \coth \kappa_1 (r_1 - r_0)$
Cylinder	$\frac{\kappa_0 r_0}{2} \frac{I_0(\kappa_0 r_0)}{I_1(\kappa_0 r_0)}$	$-\frac{\kappa_1^2 (r_1^2 - r_0^2)}{2 \kappa_1 r_0} \frac{I_1(\kappa_1 r_1) K_0(\kappa_1 r_0) - I_0(\kappa_1 r_0) K_1(\kappa_1 r_1)}{I_1(\kappa_1 r_1) K_1(\kappa_1 r_0) + I_1(\kappa_1 r_0) K_1(\kappa_1 r_1)}$
Sphere	$\frac{\kappa_0 r_0}{3} \frac{\tanh \kappa_0 r_0}{\kappa_0 r_0 - \tanh \kappa_0 r_0}$	$\frac{\kappa_1^3 (r_1^2 - r_0^2)}{3 \kappa_1^2 (r_1^2 - r_0^2)} \frac{\kappa_1 r_0 \coth \kappa_1 (r_1 - r_0)}{\kappa_1 r_0 + \coth \kappa_1 (r_1 - r_0)}$

The structure of the thermal utilization formulas, as pointed out by J. A. Wheeler, is easily understood. If the diffusion coefficient in the moderator were infinite (Figure 3) then there could be no gradient of neutrons in the moderator, i.e., the neutron density there would be uniform. In this case $\kappa_1 = 0$, and as may be easily verified, $E = 1$.

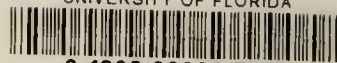
Thus the quantity $1 + \frac{N_1 \sigma_{a1} V_1}{N_0 \sigma_{a0} V_0} F$ represents the reciprocal of the thermal utilization if the neutron density throughout the moderator were just the same as its value at the interface between moderator and metal. This can also be seen if we observe that the quantity F according to (16) is the ratio of the neutron density at the interface to the average inside the lump. The quantity $\frac{N_1 \sigma_{a1} V_1}{N_0 \sigma_{a0} V_0} F$ is therefore the ratio of the absorptions in moderator and uranium if the neutron density in the moderator is uniform and equal to its value at the uranium surface. This quantity is often called the "relative absorption".

Actually the diffusion coefficient is finite and therefore the neutron density in the moderator is higher than it is in the uranium. This causes an additional absorption of neutrons in the moderator and



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